

Abstract Submitted  
for the MAR10 Meeting of  
The American Physical Society

**Sodium doped TiOCl as a realization of a multiband ionic Hubbard model**<sup>1</sup> HARALD O. JESCHKE, YU-ZHONG ZHANG, KATERYNA FOYEVTSOVA, Institut fuer Theoretische Physik, Universitaet Frankfurt, MARTIN U. SCHMIDT, Institut fuer Anorganische und Analytische Chemie, Universitaet Frankfurt, ROSER VALENTI, Institut fuer Theoretische Physik, Universitaet Frankfurt — Using first principles molecular dynamics simulations, we investigate the effect of Na intercalation in the layered Mott insulator TiOCl. In agreement with recent photoemission experiments, we find that the system remains insulating for all studied Na concentrations. Our calculations also explain the evolution of the spectral weight upon Na doping. This is possible due to a prediction of the Na-doped superlattice structures. In the search for alternatives to metallize TiOCl, we also carried out simulations of substitutions of O by F, Cl by S, or Ti by V (or Sc), respectively, but all resulting structures turn out to be insulating. We propose a description in terms of a multiorbital ionic Hubbard model in a quasi-two-dimensional lattice and discuss the nature of the insulating state under doping. Finally, a different route for metallizing TiOCl by doping is proposed.

<sup>1</sup>This work was supported by the Deutsche Forschungsgemeinschaft through TRR/SFB 49, FOR 412 and Emmy Noether programs.

Harald O. Jeschke  
Institut fuer Theoretische Physik, Universitaet Frankfurt

Date submitted: 19 Nov 2009

Electronic form version 1.4